



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2016 – 01:11 PM EST

PDB ID : 5EGF
Title : The crystal structure of SeMet-CT
Authors : Zhang, J.R.; Tang, Y.; Zhou, J.H.
Deposited on : 2015-10-27
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

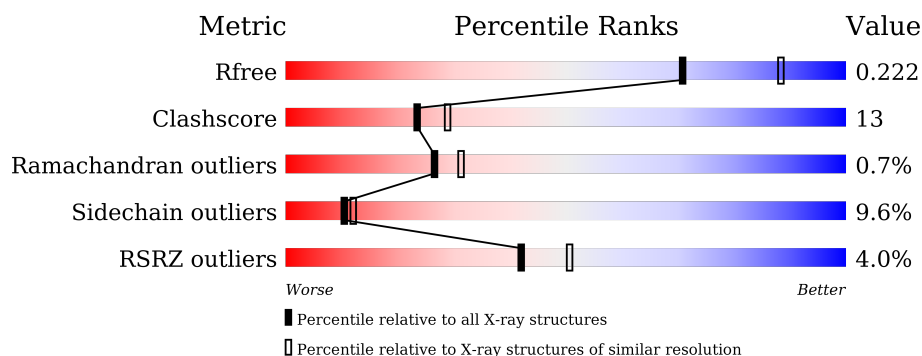
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	486	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	486	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	486	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	503	-	-	-	X
2	EDO	A	504	-	-	X	X
2	EDO	A	505	-	-	-	X
2	EDO	B	501	-	-	-	X
2	EDO	B	502	-	-	X	-
2	EDO	B	503	-	-	-	X
2	EDO	B	505	-	-	-	X
2	EDO	B	506	-	-	X	X
2	EDO	B	508	-	-	X	X
2	EDO	B	511	-	-	-	X
2	EDO	C	501	-	-	X	-
2	EDO	C	502	-	-	-	X
2	EDO	C	504	-	-	X	X
2	EDO	C	505	-	-	-	X
2	EDO	C	508	-	-	-	X
2	EDO	D	502	-	-	-	X
2	EDO	D	504	-	-	-	X
2	EDO	D	505	-	-	-	X
3	C8E	A	508	-	-	X	X
3	C8E	B	512	-	-	X	X
3	C8E	C	509	-	-	X	-
3	C8E	D	511	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14879 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TqaA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	1	0
			3529	2257	609	650	7	6			
1	B	443	Total	C	N	O	S	Se	0	1	0
			3527	2252	609	653	7	6			
1	C	444	Total	C	N	O	S	Se	0	2	0
			3544	2265	612	654	7	6			
1	D	442	Total	C	N	O	S	Se	0	1	0
			3529	2257	609	650	7	6			

There are 32 discrepancies between the modelled and reference sequences:

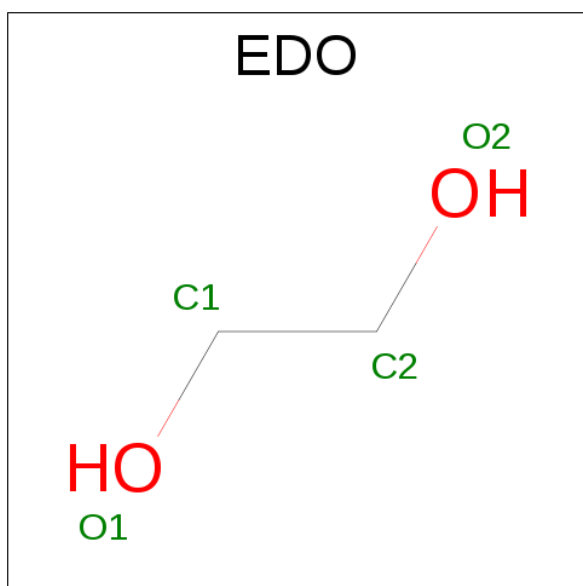
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	expression tag	UNP F1CWE4
A	3	HIS	-	expression tag	UNP F1CWE4
A	4	HIS	-	expression tag	UNP F1CWE4
A	5	HIS	-	expression tag	UNP F1CWE4
A	6	HIS	-	expression tag	UNP F1CWE4
A	7	HIS	-	expression tag	UNP F1CWE4
A	35	ALA	LYS	engineered mutation	UNP F1CWE4
A	36	ALA	GLU	engineered mutation	UNP F1CWE4
B	2	HIS	-	expression tag	UNP F1CWE4
B	3	HIS	-	expression tag	UNP F1CWE4
B	4	HIS	-	expression tag	UNP F1CWE4
B	5	HIS	-	expression tag	UNP F1CWE4
B	6	HIS	-	expression tag	UNP F1CWE4
B	7	HIS	-	expression tag	UNP F1CWE4
B	35	ALA	LYS	engineered mutation	UNP F1CWE4
B	36	ALA	GLU	engineered mutation	UNP F1CWE4
C	2	HIS	-	expression tag	UNP F1CWE4
C	3	HIS	-	expression tag	UNP F1CWE4
C	4	HIS	-	expression tag	UNP F1CWE4
C	5	HIS	-	expression tag	UNP F1CWE4
C	6	HIS	-	expression tag	UNP F1CWE4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	HIS	-	expression tag	UNP F1CWE4
C	35	ALA	LYS	engineered mutation	UNP F1CWE4
C	36	ALA	GLU	engineered mutation	UNP F1CWE4
D	2	HIS	-	expression tag	UNP F1CWE4
D	3	HIS	-	expression tag	UNP F1CWE4
D	4	HIS	-	expression tag	UNP F1CWE4
D	5	HIS	-	expression tag	UNP F1CWE4
D	6	HIS	-	expression tag	UNP F1CWE4
D	7	HIS	-	expression tag	UNP F1CWE4
D	35	ALA	LYS	engineered mutation	UNP F1CWE4
D	36	ALA	GLU	engineered mutation	UNP F1CWE4

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

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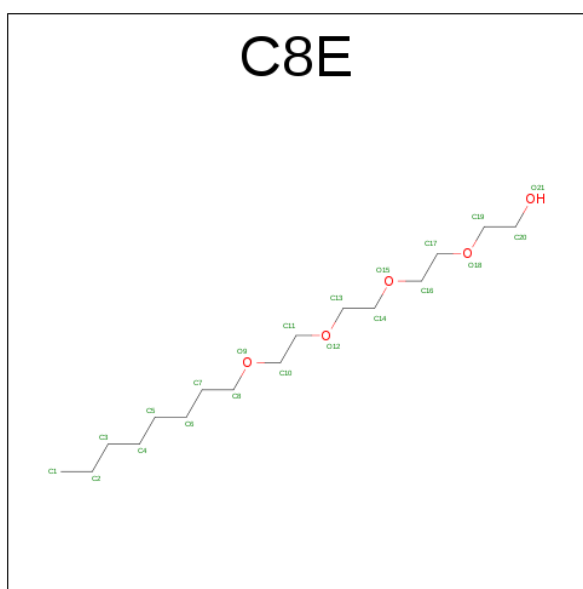
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 16 5	0	0
3	B	1	Total C O 21 16 5	0	0
3	C	1	Total C O 21 16 5	0	0

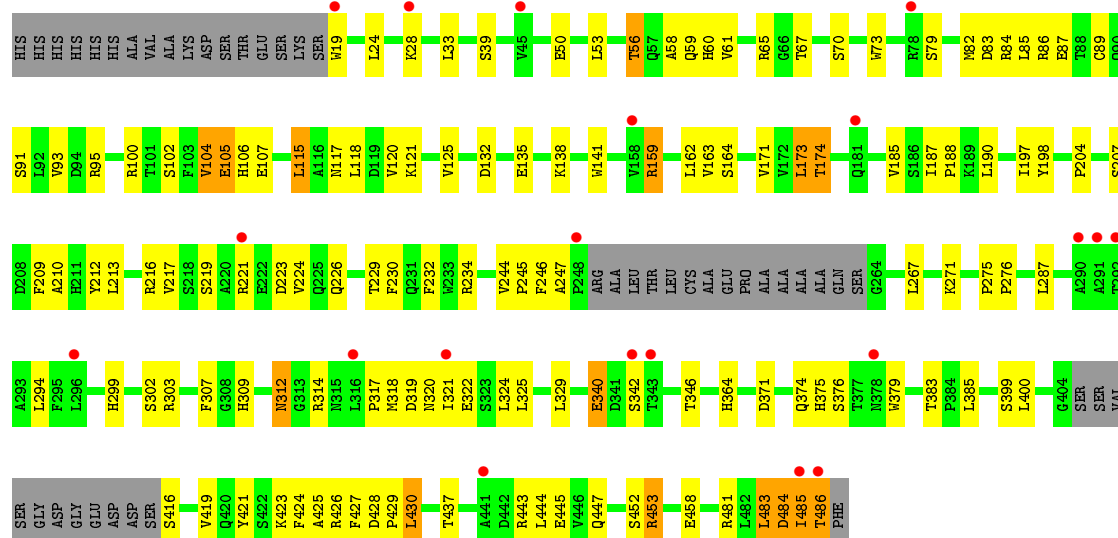
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	179	Total	O	0	0
			179	179		
4	C	134	Total	O	0	0
			134	134		
4	D	98	Total	O	0	0
			98	98		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.60 Å 100.28 Å 128.23 Å 90.00° 100.18° 90.00°	Depositor
Resolution (Å)	29.75 – 2.29 29.75 – 2.29	Depositor EDS
% Data completeness (in resolution range)	85.4 (29.75-2.29) 85.1 (29.75-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.29 Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.225 , 0.266 0.214 , 0.222	Depositor DCC
R_{free} test set	1696 reflections (1.65%)	DCC
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14879	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C8E, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/3626	0.61	0/4946
1	B	0.50	0/3623	0.63	1/4941 (0.0%)
1	C	0.44	0/3645	0.58	0/4970
1	D	0.41	0/3626	0.57	0/4946
All	All	0.45	0/14520	0.60	1/19803 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ALA	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	484	ASP	Peptide
1	B	247	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3529	0	3454	89	0
1	B	3527	0	3452	78	0
1	C	3544	0	3466	100	0
1	D	3529	0	3454	96	0
2	A	28	0	42	9	0
2	B	40	0	60	20	0
2	C	32	0	48	16	0
2	D	40	0	60	9	0
3	A	21	0	34	9	0
3	B	21	0	34	16	0
3	C	21	0	34	12	0
3	D	21	0	34	9	0
4	A	115	0	0	2	0
4	B	179	0	0	6	0
4	C	134	0	0	9	0
4	D	98	0	0	5	0
All	All	14879	0	14172	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:EDO:H11	3:B:512:C8E:H13	1.34	1.08
2:C:501:EDO:H21	3:C:509:C8E:H81	1.36	1.02
2:B:502:EDO:H22	3:B:512:C8E:H32	1.44	0.99
1:B:95:ARG:HH21	1:B:203:LEU:HB3	1.25	0.98
1:D:56:THR:HG22	1:D:59:GLN:H	1.30	0.97
1:B:267:LEU:HB2	2:B:506:EDO:H11	1.50	0.93
3:A:508:C8E:H21	1:D:246:PHE:H	1.36	0.90
1:B:472:THR:O	1:B:476:THR:HG23	1.74	0.87
1:D:485:ILE:HD12	1:D:486:THR:HG22	1.59	0.84
3:A:508:C8E:H12	3:D:511:C8E:H142	1.57	0.84
2:B:502:EDO:C1	3:B:512:C8E:H13	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:O	1:D:299:HIS:HD2	1.63	0.81
1:C:303:ARG:H	2:C:505:EDO:H11	1.45	0.80
1:D:483:LEU:HD12	1:D:484:ASP:HB2	1.64	0.80
1:A:289:LYS:NZ	1:A:309:HIS:HD2	1.79	0.80
1:B:267:LEU:CB	2:B:506:EDO:H11	2.12	0.79
1:A:151:VAL:H	2:A:504:EDO:H21	1.47	0.78
1:C:20:GLU:N	1:C:23:SER:HG	1.82	0.77
1:B:95:ARG:NH2	1:B:203:LEU:HB3	2.00	0.75
1:C:307:PHE:HA	2:C:502:EDO:H12	1.68	0.75
1:B:202:PRO:HD2	4:B:756:HOH:O	1.86	0.74
1:C:366[B]:HIS:HD2	4:C:609:HOH:O	1.69	0.73
1:B:314:ARG:NH1	1:B:328:THR:OG1	2.23	0.72
1:B:460:ALA:CB	2:B:506:EDO:H12	2.20	0.72
1:C:312:ASN:HD22	1:C:313:GLY:N	1.87	0.72
1:A:141:TRP:HA	1:A:145:ASP:HB2	1.72	0.71
1:B:23:SER:O	4:B:601:HOH:O	2.07	0.71
1:C:229:THR:HG21	1:C:367:VAL:HG11	1.72	0.71
1:C:187:ILE:HG22	1:C:188:PRO:HD3	1.72	0.71
1:D:73:TRP:CZ3	1:D:421:TYR:HB2	2.25	0.71
1:A:25:SER:HB3	1:A:52:LEU:HD22	1.73	0.71
2:B:502:EDO:C2	3:B:512:C8E:H32	2.19	0.71
1:D:53:LEU:HD22	1:D:213:LEU:HD12	1.73	0.70
1:A:151:VAL:N	2:A:504:EDO:H21	2.07	0.70
1:D:187:ILE:CG2	1:D:188:PRO:HD3	2.22	0.69
1:D:187:ILE:HG22	1:D:188:PRO:HD3	1.73	0.69
1:B:33:LEU:HD22	1:B:106:HIS:HD2	1.55	0.69
1:B:387:LEU:HB3	2:B:508:EDO:H11	1.73	0.68
1:A:318:MSE:HE3	1:A:321:ILE:HD13	1.75	0.68
1:D:223:ASP:HB3	1:D:226:GLN:CD	2.13	0.68
1:A:299:HIS:HB3	3:D:511:C8E:H161	1.76	0.68
1:D:445:GLU:HG2	1:D:447:GLN:HE21	1.59	0.67
2:C:501:EDO:H21	3:C:509:C8E:C8	2.20	0.67
2:B:502:EDO:H22	3:B:512:C8E:C3	2.21	0.67
1:D:385:LEU:H	2:D:508:EDO:H21	1.60	0.67
1:A:287:LEU:HD13	1:A:471:ILE:HG23	1.76	0.66
1:D:312:ASN:HD22	1:D:314:ARG:H	1.43	0.66
1:B:56:THR:HB	2:B:505:EDO:H22	1.76	0.66
1:B:307:PHE:HA	2:B:508:EDO:H12	1.77	0.66
2:C:501:EDO:O2	3:C:509:C8E:H102	1.96	0.66
1:D:174:THR:HG21	4:D:635:HOH:O	1.95	0.66
1:C:312:ASN:C	1:C:312:ASN:HD22	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:508:C8E:H191	1:D:299:HIS:HB3	1.78	0.65
1:C:212:TYR:CE2	1:C:216:ARG:HD2	2.31	0.65
1:A:289:LYS:HZ3	1:A:309:HIS:HD2	1.43	0.65
1:A:436:PHE:HB2	1:A:447:GLN:HB2	1.79	0.64
1:D:209:PHE:O	1:D:212:TYR:HB3	1.97	0.64
1:C:147:PRO:HG3	2:C:506:EDO:H22	1.78	0.64
1:A:319:ASP:O	1:A:320:ASN:HB2	1.98	0.64
1:A:190:LEU:HD12	1:A:325:LEU:HD21	1.81	0.63
1:A:312:ASN:HD22	1:A:314:ARG:H	1.46	0.63
1:B:141:TRP:HA	1:B:145:ASP:HB2	1.80	0.63
1:D:33:LEU:HD13	1:D:106:HIS:CD2	2.34	0.63
1:A:28:LYS:HD3	1:A:28:LYS:N	2.14	0.63
1:A:73:TRP:CZ3	1:A:421:TYR:HB2	2.34	0.62
1:B:60:HIS:CE1	1:B:64:LYS:HE2	2.34	0.62
1:D:322:GLU:CD	1:D:322:GLU:H	2.03	0.62
1:A:244:VAL:O	1:D:299:HIS:CD2	2.50	0.62
3:A:508:C8E:H21	1:D:246:PHE:N	2.11	0.62
1:B:426:ARG:HA	2:B:504:EDO:H21	1.81	0.62
1:B:212:TYR:CE2	1:B:216:ARG:HD2	2.35	0.61
1:B:244:VAL:O	1:C:299:HIS:HD2	1.83	0.61
1:C:65:ARG:NH2	1:C:430:LEU:HD22	2.15	0.61
1:D:121:LYS:HB3	4:D:636:HOH:O	1.99	0.61
1:C:146:TRP:CG	1:C:147:PRO:HD3	2.36	0.61
1:B:248:PRO:HG3	4:B:699:HOH:O	2.01	0.60
1:A:187:ILE:HG22	1:A:188:PRO:HD3	1.82	0.60
3:B:512:C8E:H162	3:C:509:C8E:H101	1.84	0.60
1:D:314:ARG:NH2	1:D:324:LEU:O	2.35	0.60
1:C:331:PHE:HB2	2:C:504:EDO:C2	2.31	0.60
1:B:79:SER:HG	1:B:415:SER:N	1.98	0.60
1:B:297:SER:HB2	1:B:302:SER:O	2.01	0.59
1:A:156:LEU:O	2:A:503:EDO:H22	2.01	0.59
2:C:501:EDO:H11	3:C:509:C8E:H191	1.83	0.59
3:B:512:C8E:H171	1:C:299:HIS:HB3	1.84	0.59
1:D:294:LEU:HD21	1:D:485:ILE:HG21	1.84	0.59
1:B:229:THR:HA	1:B:364:HIS:ND1	2.18	0.59
1:C:215[B]:HIS:CG	1:C:318:MSE:HE2	2.38	0.59
1:C:215[A]:HIS:CG	1:C:318:MSE:HE2	2.38	0.59
1:A:146:TRP:CD2	1:A:147:PRO:HD3	2.38	0.59
1:C:93:VAL:HG13	1:C:100:ARG:HG2	1.84	0.58
3:A:508:C8E:H11	3:D:511:C8E:H62	1.85	0.58
1:A:264:GLY:HA2	1:A:453:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLY:HA2	4:C:640:HOH:O	2.02	0.58
1:A:477:ASP:OD1	1:A:479:THR:HB	2.02	0.58
1:D:95:ARG:NH2	1:D:204:PRO:O	2.35	0.58
1:B:485:ILE:HG23	1:B:486:THR:H	1.68	0.58
1:A:187:ILE:CG2	1:A:188:PRO:HD3	2.33	0.58
1:B:267:LEU:HB2	2:B:506:EDO:C1	2.32	0.57
1:C:473:LYS:HZ3	1:C:485:ILE:H	1.49	0.57
1:B:348:MSE:CE	1:B:478:PRO:HB2	2.34	0.57
1:D:485:ILE:HD12	1:D:486:THR:CG2	2.33	0.57
2:C:501:EDO:H11	3:C:509:C8E:H171	1.85	0.57
1:C:466:ASN:O	1:C:470:ILE:HG13	2.04	0.57
1:A:234:ARG:N	1:A:376:SER:HB3	2.20	0.57
1:C:270:PHE:CD2	1:C:447:GLN:HG2	2.40	0.57
1:C:83:ASP:O	1:C:87:GLU:HG3	2.04	0.57
1:A:158:VAL:HA	1:A:176:GLN:O	2.04	0.57
2:C:501:EDO:C2	3:C:509:C8E:H81	2.23	0.57
1:D:83:ASP:O	1:D:87:GLU:HG3	2.05	0.57
3:B:512:C8E:H11	2:C:501:EDO:O1	2.05	0.56
1:D:275:PRO:HD3	1:D:443:ARG:HA	1.87	0.56
1:D:379:TRP:N	1:D:379:TRP:CD1	2.71	0.56
3:B:512:C8E:H71	3:C:509:C8E:H22	1.87	0.56
1:C:303:ARG:HG2	1:C:338:PHE:HB2	1.87	0.56
1:C:473:LYS:NZ	1:C:485:ILE:H	2.02	0.56
1:D:303:ARG:HG3	4:D:685:HOH:O	2.05	0.56
1:B:86:ARG:O	1:B:89:CYS:HB2	2.06	0.56
1:C:297:SER:HB2	1:C:302:SER:O	2.04	0.56
1:B:270:PHE:CD2	1:B:447:GLN:HG2	2.41	0.56
1:B:250:ALA:O	1:C:458:GLU:HG3	2.05	0.55
1:A:34:HIS:HB2	1:A:49:LEU:HD22	1.87	0.55
1:A:65:ARG:CZ	1:A:430:LEU:HD22	2.36	0.55
1:C:155:SER:HB3	4:C:608:HOH:O	2.06	0.55
1:A:28:LYS:CD	1:A:28:LYS:N	2.69	0.55
1:C:331:PHE:HB2	2:C:504:EDO:H21	1.88	0.55
1:C:400:LEU:HB3	1:C:419:VAL:HG11	1.88	0.55
1:D:245:PRO:HA	3:D:511:C8E:H142	1.89	0.55
1:C:91:SER:O	1:C:94:ASP:HB2	2.07	0.55
1:A:146:TRP:CG	1:A:147:PRO:HD3	2.42	0.54
1:D:307:PHE:HA	2:D:502:EDO:H21	1.89	0.54
1:C:65:ARG:CZ	1:C:430:LEU:HD22	2.37	0.54
1:B:296:LEU:HD11	1:B:387:LEU:HD23	1.90	0.53
1:D:138:LYS:HD3	1:D:424:PHE:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:SER:HB2	1:C:141:TRP:CZ3	2.42	0.53
1:A:276:PRO:HD2	1:A:284:MSE:HE1	1.91	0.53
1:D:383:THR:HA	2:D:506:EDO:H11	1.90	0.53
1:A:340:GLU:O	1:A:341:ASP:HB3	2.08	0.53
3:B:512:C8E:H141	3:C:509:C8E:H71	1.90	0.53
1:C:112:GLN:HE22	1:C:213:LEU:HD11	1.73	0.53
1:C:21:PRO:HB2	1:C:22:PHE:HD1	1.74	0.53
1:D:65:ARG:CZ	1:D:430:LEU:HD22	2.39	0.53
3:A:508:C8E:H13	3:D:511:C8E:C1	2.40	0.52
1:A:240:ALA:HB2	1:A:335:ARG:CZ	2.39	0.52
1:C:436:PHE:HB2	1:C:447:GLN:HB2	1.91	0.52
1:A:151:VAL:H	2:A:504:EDO:C2	2.18	0.52
1:B:246:PHE:O	1:B:247:ALA:HB3	2.10	0.52
1:A:299:HIS:HD2	1:D:244:VAL:O	1.92	0.52
1:C:331:PHE:HD2	2:C:504:EDO:H22	1.73	0.52
1:C:187:ILE:CG2	1:C:188:PRO:HD3	2.39	0.52
1:D:224:VAL:HG11	1:D:375:HIS:CG	2.44	0.52
1:B:158:VAL:HA	1:B:176:GLN:O	2.10	0.52
1:C:195:ALA:HB2	1:C:400:LEU:HD12	1.91	0.52
1:D:190:LEU:HD12	1:D:325:LEU:HD21	1.92	0.52
1:D:93:VAL:HG12	1:D:100:ARG:HG3	1.91	0.52
1:A:340:GLU:O	1:A:341:ASP:CB	2.59	0.51
1:B:82:MSE:HB3	1:B:86:ARG:HH12	1.74	0.51
1:C:284:MSE:CG	1:C:391:HIS:CE1	2.93	0.51
1:C:73:TRP:CZ3	1:C:421:TYR:HB2	2.46	0.51
1:D:70:SER:HB3	1:D:424:PHE:HB2	1.92	0.51
1:A:60:HIS:NE2	1:A:110:PRO:HB3	2.26	0.51
1:B:247:ALA:HB3	1:B:248:PRO:HA	1.91	0.51
1:B:82:MSE:HB3	1:B:86:ARG:NH1	2.26	0.51
1:D:93:VAL:HG12	1:D:100:ARG:CG	2.40	0.51
1:C:271:LYS:HD3	1:C:465:ASN:OD1	2.11	0.51
1:C:52:LEU:HD23	1:C:52:LEU:C	2.31	0.51
1:A:311:VAL:HG21	1:A:365:GLU:HB2	1.92	0.51
1:B:146:TRP:CG	1:B:147:PRO:HD3	2.45	0.51
1:B:27:ILE:HD11	1:B:52:LEU:HD11	1.93	0.51
1:C:245:PRO:HB3	2:C:501:EDO:H12	1.93	0.51
1:A:28:LYS:H	1:A:28:LYS:HE3	1.74	0.50
1:A:284:MSE:H	2:A:506:EDO:H21	1.76	0.50
1:B:52:LEU:HD23	1:B:52:LEU:C	2.31	0.50
1:D:229:THR:HA	1:D:364:HIS:ND1	2.26	0.50
1:A:138:LYS:HE2	1:A:142:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:HG23	1:B:116:ALA:C	2.31	0.50
1:B:234:ARG:N	1:B:376:SER:HB3	2.27	0.50
1:B:203:LEU:N	4:B:607:HOH:O	2.41	0.50
1:A:27:ILE:HA	1:A:28:LYS:HD3	1.94	0.49
1:A:373:PHE:HA	1:A:377:THR:OG1	2.12	0.49
1:C:323:SER:HB2	4:C:638:HOH:O	2.12	0.49
1:C:93:VAL:CG1	1:C:100:ARG:HG2	2.42	0.49
1:D:329:LEU:HD21	2:D:510:EDO:H21	1.94	0.49
1:C:102:SER:HB2	1:C:154:GLY:O	2.13	0.49
1:D:427:PHE:HB2	2:D:504:EDO:H11	1.95	0.49
1:A:48:THR:HG23	1:A:117:ASN:HB2	1.95	0.49
1:D:138:LYS:HD3	1:D:424:PHE:CZ	2.47	0.49
1:C:132:ASP:OD1	1:C:133:PRO:HD2	2.13	0.49
1:C:331:PHE:CD2	2:C:504:EDO:H22	2.47	0.49
1:D:453:ARG:HD3	1:D:453:ARG:O	2.12	0.49
1:C:224:VAL:C	1:C:226:GLN:H	2.16	0.49
1:A:214:TYR:CE1	4:A:601:HOH:O	2.55	0.49
1:A:230:PHE:CZ	1:A:371:ASP:HB3	2.47	0.49
1:C:284:MSE:HG3	1:C:391:HIS:CE1	2.48	0.49
1:D:485:ILE:O	1:D:485:ILE:HG13	2.09	0.49
1:D:312:ASN:ND2	1:D:314:ARG:H	2.11	0.48
1:A:377:THR:HG22	4:A:615:HOH:O	2.13	0.48
1:A:275:PRO:HD3	1:A:443:ARG:HA	1.96	0.48
1:C:20:GLU:N	1:C:23:SER:H	2.10	0.48
1:A:289:LYS:HZ3	1:A:309:HIS:CD2	2.28	0.48
1:D:340:GLU:H	1:D:340:GLU:HG3	1.36	0.48
1:A:199:ASN:O	1:A:200:GLN:HB2	2.14	0.48
1:A:144:LYS:NZ	1:B:131:GLU:HG3	2.29	0.48
1:A:289:LYS:HZ1	1:A:309:HIS:HD2	1.55	0.48
1:C:287:LEU:HD22	1:C:471:ILE:HG23	1.96	0.48
1:C:312:ASN:ND2	1:C:314:ARG:H	2.11	0.48
1:C:80:LEU:HB3	4:C:667:HOH:O	2.13	0.48
1:A:289:LYS:HE2	1:A:309:HIS:HB2	1.96	0.48
1:B:54:PRO:HA	1:B:111:ILE:HG22	1.95	0.48
1:C:366[B]:HIS:CD2	4:C:609:HOH:O	2.55	0.47
1:D:141:TRP:HE1	2:D:503:EDO:C2	2.27	0.47
1:B:112:GLN:HE22	1:B:213:LEU:HD11	1.80	0.47
1:A:133:PRO:HB2	1:A:172:VAL:HG23	1.96	0.47
1:C:138:LYS:HD3	1:C:424:PHE:CE1	2.50	0.47
1:C:209:PHE:O	1:C:212:TYR:HB3	2.14	0.47
1:C:31:GLN:HE22	1:C:49:LEU:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:THR:HB	1:D:59:GLN:OE1	2.14	0.47
1:D:84:ARG:HG2	1:D:198:TYR:CD1	2.50	0.47
1:D:89:CYS:O	1:D:93:VAL:HG23	2.15	0.47
1:A:348:MSE:HE2	1:A:478:PRO:HB3	1.96	0.47
1:A:264:GLY:HA3	1:A:453:ARG:NH1	2.30	0.47
3:B:512:C8E:H12	3:C:509:C8E:H31	1.96	0.46
1:D:212:TYR:CE2	1:D:216:ARG:HD2	2.51	0.46
1:D:56:THR:HG22	1:D:59:GLN:N	2.14	0.46
1:C:173:LEU:HD22	1:C:174:THR:N	2.31	0.46
1:C:402:LEU:HD12	1:C:402:LEU:HA	1.74	0.46
1:D:125:VAL:HB	1:D:163:VAL:HG13	1.98	0.46
1:A:229:THR:HA	1:A:364:HIS:ND1	2.30	0.46
1:A:82:MSE:O	1:A:86:ARG:HG3	2.15	0.46
1:D:232:PHE:C	1:D:232:PHE:CD1	2.86	0.46
1:D:346:THR:HA	1:D:481:ARG:HA	1.98	0.46
1:B:199:ASN:HB3	4:B:616:HOH:O	2.15	0.46
1:D:229:THR:HG23	1:D:364:HIS:HB3	1.97	0.46
1:B:185:VAL:HG12	4:B:722:HOH:O	2.15	0.46
3:A:508:C8E:H13	3:D:511:C8E:H12	1.98	0.46
3:B:512:C8E:H41	3:C:509:C8E:H22	1.97	0.46
1:D:425:ALA:H	2:D:503:EDO:H21	1.81	0.46
1:A:312:ASN:ND2	1:A:314:ARG:H	2.11	0.46
1:B:307:PHE:CB	2:B:508:EDO:H12	2.45	0.46
1:D:24:LEU:HD11	1:D:217:VAL:HG21	1.96	0.46
1:B:58:ALA:HB2	2:B:505:EDO:H11	1.98	0.45
1:C:223:ASP:HB3	1:C:226:GLN:OE1	2.17	0.45
1:C:225:GLN:H	1:C:225:GLN:CD	2.19	0.45
1:B:229:THR:HG21	1:B:367:VAL:HG11	1.98	0.45
1:D:425:ALA:N	2:D:503:EDO:H21	2.32	0.45
1:D:56:THR:HG23	4:D:657:HOH:O	2.17	0.45
1:A:477:ASP:OD2	1:A:480:ALA:HB2	2.17	0.45
1:D:318:MSE:HE3	1:D:321:ILE:HD13	1.98	0.45
1:B:193:ASP:O	1:B:197:ILE:HG13	2.16	0.45
1:B:347:VAL:O	1:B:351:LEU:HG	2.17	0.45
1:D:164:SER:OG	1:D:171:VAL:HG22	2.17	0.45
1:A:43:ILE:HB	1:A:44:PRO:HD2	1.99	0.45
1:C:79:SER:HG	1:C:415:SER:N	2.15	0.45
1:D:82:MSE:O	1:D:86:ARG:HG3	2.17	0.45
1:B:307:PHE:CA	2:B:508:EDO:H12	2.47	0.45
1:B:48:THR:HG23	1:B:116:ALA:HB3	1.98	0.44
1:B:91:SER:HB3	1:B:197:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:TRP:CZ2	1:D:159:ARG:HB3	2.52	0.44
1:C:287:LEU:O	1:C:287:LEU:HD23	2.17	0.44
1:A:374:GLN:HB2	1:A:374:GLN:HE21	1.56	0.44
1:C:379:TRP:CD1	1:C:379:TRP:N	2.85	0.44
1:D:267:LEU:HG	1:D:452:SER:HB3	2.00	0.44
1:A:124:GLU:O	1:B:125:VAL:HA	2.17	0.44
1:B:223:ASP:OD2	1:B:226:GLN:HG3	2.17	0.44
1:A:396:LEU:HD13	1:A:440:HIS:CE1	2.53	0.44
1:A:473:LYS:HZ1	1:A:485:ILE:HG13	1.82	0.44
1:A:82:MSE:HB3	1:A:82:MSE:HE3	1.90	0.44
1:B:125:VAL:HB	1:B:163:VAL:HG13	2.00	0.44
1:C:200:GLN:HB3	1:C:200:GLN:HE21	1.66	0.43
1:D:223:ASP:HB3	1:D:226:GLN:OE1	2.18	0.43
1:C:229:THR:HG21	1:C:367:VAL:CG1	2.46	0.43
1:D:287:LEU:HD23	1:D:287:LEU:O	2.18	0.43
1:D:234:ARG:N	1:D:376:SER:HB3	2.34	0.43
1:A:132:ASP:OD1	1:A:133:PRO:HD2	2.18	0.43
1:B:392:GLN:HA	1:B:392:GLN:OE1	2.17	0.43
1:C:158:VAL:HA	1:C:176:GLN:O	2.18	0.43
1:D:162:LEU:HD12	1:D:162:LEU:HA	1.84	0.43
1:A:344:ASP:HA	1:A:481:ARG:HD2	1.99	0.43
1:C:125:VAL:HB	1:C:163:VAL:HG13	2.00	0.43
1:D:428:ASP:HA	1:D:429:PRO:HD2	1.90	0.43
1:B:208:ASP:HB3	1:B:210:ALA:H	1.83	0.43
2:B:502:EDO:H12	3:B:512:C8E:O15	2.19	0.43
1:D:426:ARG:HA	2:D:507:EDO:H21	2.00	0.43
1:A:158:VAL:O	1:A:158:VAL:HG12	2.18	0.43
1:C:248:PRO:HB2	1:C:453:ARG:HD3	2.00	0.43
1:C:481:ARG:NH2	1:C:483:LEU:HD23	2.33	0.43
1:A:390:GLN:HB2	1:A:390:GLN:HE21	1.73	0.43
1:C:28:LYS:HB3	1:C:28:LYS:HE2	1.73	0.43
1:B:455:LEU:HD13	3:B:512:C8E:H42	2.00	0.43
1:C:21:PRO:O	1:C:22:PHE:HB2	2.18	0.43
1:C:294:LEU:HD22	1:C:474:PHE:CZ	2.54	0.43
1:D:173:LEU:HD22	1:D:174:THR:H	1.83	0.43
1:A:159:ARG:CZ	2:A:503:EDO:H21	2.48	0.43
1:A:356:THR:O	1:A:360:ARG:HG3	2.19	0.43
1:C:318:MSE:HG2	1:C:321:ILE:HB	2.00	0.43
1:A:318:MSE:HB3	1:A:321:ILE:HB	1.99	0.43
1:A:339:PRO:O	1:A:340:GLU:C	2.57	0.42
1:C:106:HIS:O	1:C:107:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD11	1:C:387:LEU:HD23	2.01	0.42
1:D:190:LEU:HD23	1:D:190:LEU:C	2.39	0.42
3:A:508:C8E:H31	3:D:511:C8E:H13	2.01	0.42
1:A:341:ASP:C	1:A:343:THR:H	2.23	0.42
1:B:450:ALA:O	2:B:506:EDO:H22	2.18	0.42
1:D:210:ALA:O	1:D:213:LEU:N	2.51	0.42
1:D:93:VAL:HG21	1:D:120:VAL:HG21	2.01	0.42
1:B:348:MSE:HE1	1:B:478:PRO:HB2	2.00	0.42
1:C:137:CYS:SG	1:C:163:VAL:HG21	2.60	0.42
1:C:275:PRO:HA	1:C:276:PRO:HD3	1.82	0.42
1:C:31:GLN:NE2	1:C:49:LEU:HB3	2.34	0.42
1:D:321:ILE:HG23	1:D:322:GLU:N	2.33	0.42
1:A:485:ILE:HA	1:A:485:ILE:HD12	1.79	0.42
1:A:206:THR:HG23	2:A:505:EDO:H11	2.02	0.42
1:B:338:PHE:CE2	1:B:350:LEU:HD13	2.53	0.42
1:B:104:VAL:HG13	1:B:105:GLU:N	2.34	0.42
1:D:104:VAL:HG13	1:D:105:GLU:N	2.35	0.42
1:A:303:ARG:HB2	1:A:338:PHE:HB2	2.02	0.42
1:C:241:LYS:NZ	4:C:606:HOH:O	2.44	0.42
2:C:501:EDO:C1	3:C:509:C8E:H171	2.48	0.42
1:D:118:LEU:HA	1:D:118:LEU:HD12	1.87	0.42
1:D:319:ASP:O	1:D:320:ASN:HB2	2.20	0.42
1:D:58:ALA:O	1:D:61:VAL:HB	2.20	0.42
1:A:151:VAL:HB	2:A:504:EDO:H22	2.01	0.42
1:A:264:GLY:CA	1:A:453:ARG:HD2	2.50	0.42
1:B:436:PHE:HB2	1:B:447:GLN:HB2	2.02	0.42
1:C:107:GLU:HG3	4:C:645:HOH:O	2.19	0.42
1:C:95:ARG:NH1	1:C:203:LEU:HD13	2.35	0.42
1:D:132:ASP:OD2	1:D:135:GLU:HG3	2.20	0.42
1:A:95:ARG:HD3	1:A:193:ASP:OD2	2.20	0.41
1:D:173:LEU:HD22	1:D:174:THR:N	2.35	0.41
1:D:234:ARG:HE	1:D:376:SER:HA	1.84	0.41
1:A:144:LYS:HZ1	1:B:131:GLU:HG3	1.85	0.41
1:B:91:SER:O	1:B:94:ASP:HB2	2.20	0.41
1:D:230:PHE:CZ	1:D:371:ASP:HB3	2.55	0.41
1:A:159:ARG:NH2	2:A:503:EDO:H21	2.36	0.41
1:A:473:LYS:N	1:A:473:LYS:HD3	2.36	0.41
1:B:245:PRO:HG3	3:B:512:C8E:H82	2.02	0.41
1:C:284:MSE:HG2	1:C:391:HIS:CE1	2.55	0.41
1:D:275:PRO:HA	1:D:276:PRO:HD3	1.87	0.41
1:D:400:LEU:HB3	1:D:419:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:O	1:C:299:HIS:CD2	2.70	0.41
1:B:437:THR:HG22	1:B:446:VAL:HG22	2.02	0.41
1:C:417:LEU:HD12	1:C:417:LEU:HA	1.82	0.41
1:A:299:HIS:CD2	1:D:244:VAL:O	2.72	0.41
1:B:267:LEU:HB3	2:B:506:EDO:H11	1.96	0.41
1:C:402:LEU:O	1:C:403:ARG:HB3	2.20	0.41
1:B:31:GLN:HB3	1:B:31:GLN:HE21	1.72	0.41
1:B:146:TRP:CD2	1:B:147:PRO:HD3	2.56	0.41
1:C:187:ILE:N	1:C:188:PRO:CD	2.83	0.41
1:B:60:HIS:CE1	1:B:110:PRO:HG3	2.55	0.41
1:B:109:HIS:N	1:B:109:HIS:ND1	2.68	0.41
1:C:156:LEU:O	4:C:601:HOH:O	2.22	0.41
1:C:161:THR:HB	1:C:174:THR:OG1	2.21	0.41
1:D:100:ARG:HD2	1:D:115:LEU:O	2.20	0.41
1:D:91:SER:HB2	1:D:197:ILE:HG21	2.02	0.41
1:D:39:SER:HA	4:D:642:HOH:O	2.20	0.41
1:A:101:THR:CG2	1:A:112:GLN:HB2	2.51	0.41
1:B:190:LEU:HD23	1:B:190:LEU:C	2.41	0.41
1:C:229:THR:HA	1:C:364:HIS:ND1	2.36	0.41
1:D:85:LEU:HA	1:D:85:LEU:HD23	1.95	0.41
1:B:133:PRO:HB2	1:B:172:VAL:HG23	2.03	0.40
1:C:287:LEU:CD2	1:C:471:ILE:HG23	2.50	0.40
1:A:359:THR:HA	1:A:362:LEU:HG	2.03	0.40
1:C:104:VAL:O	1:C:110:PRO:HA	2.21	0.40
1:C:93:VAL:HG21	1:C:120:VAL:HG21	2.03	0.40
1:C:463:LEU:O	1:C:467:ILE:HG12	2.21	0.40
1:A:348:MSE:HE2	1:A:348:MSE:HB2	2.00	0.40
1:B:31:GLN:HG2	1:B:31:GLN:H	1.64	0.40
1:C:27:ILE:HD11	1:C:52:LEU:HD11	2.03	0.40
1:C:79:SER:HB2	1:C:405:SER:N	2.37	0.40
1:D:141:TRP:CE2	1:D:424:PHE:HB3	2.56	0.40
1:A:265:GLN:O	1:A:265:GLN:HG2	2.21	0.40
1:A:444:LEU:HD23	1:A:444:LEU:HA	1.75	0.40
1:B:56:THR:CB	2:B:505:EDO:H22	2.49	0.40
1:C:224:VAL:HG11	1:C:375:HIS:CG	2.56	0.40
1:D:245:PRO:HB3	3:D:511:C8E:H62	2.03	0.40
3:B:512:C8E:H71	3:B:512:C8E:H41	1.97	0.40
1:D:106:HIS:CE1	1:D:107:GLU:HG3	2.57	0.40
3:A:508:C8E:C1	3:D:511:C8E:H32	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/486 (90%)	410 (94%)	24 (6%)	3 (1%)	26	31
1	B	438/486 (90%)	413 (94%)	21 (5%)	4 (1%)	21	24
1	C	440/486 (90%)	415 (94%)	22 (5%)	3 (1%)	26	31
1	D	437/486 (90%)	412 (94%)	22 (5%)	3 (1%)	26	31
All	All	1752/1944 (90%)	1650 (94%)	89 (5%)	13 (1%)	26	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	ASP
1	B	247	ALA
1	B	249	ARG
1	D	247	ALA
1	B	485	ILE
1	C	108	GLY
1	C	144	LYS
1	C	200	GLN
1	A	279	PRO
1	D	484	ASP
1	A	430	LEU
1	B	248	PRO
1	D	317	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/424 (94%)	357 (90%)	40 (10%)	9	11
1	B	398/424 (94%)	366 (92%)	32 (8%)	15	18
1	C	400/424 (94%)	357 (89%)	43 (11%)	8	9
1	D	397/424 (94%)	360 (91%)	37 (9%)	11	13
All	All	1592/1696 (94%)	1440 (90%)	152 (10%)	10	12

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	LYS
1	A	53	LEU
1	A	60	HIS
1	A	79	SER
1	A	83	ASP
1	A	95	ARG
1	A	102	SER
1	A	104	VAL
1	A	105	GLU
1	A	115	LEU
1	A	117	ASN
1	A	162	LEU
1	A	170	HIS
1	A	173	LEU
1	A	185	VAL
1	A	216	ARG
1	A	219	SER
1	A	225	GLN
1	A	238	ASP
1	A	265	GLN
1	A	274	VAL
1	A	286	THR
1	A	287	LEU
1	A	302	SER
1	A	312	ASN
1	A	318	MSE
1	A	342	SER
1	A	343	THR
1	A	344	ASP
1	A	374	GLN
1	A	377	THR
1	A	399	SER

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	437	THR
1	A	442	ASP
1	A	444	LEU
1	A	473	LYS
1	A	483	LEU
1	A	485	ILE
1	B	31	GLN
1	B	45	VAL
1	B	48	THR
1	B	78	ARG
1	B	79	SER
1	B	100	ARG
1	B	102	SER
1	B	104	VAL
1	B	106	HIS
1	B	107	GLU
1	B	109	HIS
1	B	115	LEU
1	B	117	ASN
1	B	118	LEU
1	B	121	LYS
1	B	164	SER
1	B	170	HIS
1	B	173	LEU
1	B	185	VAL
1	B	218	SER
1	B	221	ARG
1	B	241	LYS
1	B	249	ARG
1	B	287	LEU
1	B	309	HIS
1	B	397	SER
1	B	415	SER
1	B	418	ASP
1	B	430	LEU
1	B	473	LYS
1	B	482	LEU
1	B	485	ILE
1	C	20	GLU
1	C	27	ILE
1	C	31	GLN

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Mol	Chain	Res	Type
1	C	45	VAL
1	C	79	SER
1	C	83	ASP
1	C	84	ARG
1	C	85	LEU
1	C	95	ARG
1	C	102	SER
1	C	104	VAL
1	C	109	HIS
1	C	115	LEU
1	C	155	SER
1	C	164	SER
1	C	173	LEU
1	C	185	VAL
1	C	189	LYS
1	C	200	GLN
1	C	201	THR
1	C	225	GLN
1	C	265	GLN
1	C	280	SER
1	C	309	HIS
1	C	312	ASN
1	C	323	SER
1	C	324	LEU
1	C	345	TRP
1	C	374	GLN
1	C	402	LEU
1	C	403	ARG
1	C	415	SER
1	C	417	LEU
1	C	418	ASP
1	C	423	LYS
1	C	430	LEU
1	C	443	ARG
1	C	444	LEU
1	C	453	ARG
1	C	468	SER
1	C	482	LEU
1	C	483	LEU
1	C	487	PHE
1	D	19	TRP
1	D	28	LYS

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Mol	Chain	Res	Type
1	D	50	GLU
1	D	56	THR
1	D	60	HIS
1	D	67	THR
1	D	79	SER
1	D	102	SER
1	D	104	VAL
1	D	105	GLU
1	D	115	LEU
1	D	117	ASN
1	D	159	ARG
1	D	173	LEU
1	D	174	THR
1	D	185	VAL
1	D	207	SER
1	D	219	SER
1	D	221	ARG
1	D	271	LYS
1	D	302	SER
1	D	309	HIS
1	D	312	ASN
1	D	340	GLU
1	D	342	SER
1	D	374	GLN
1	D	399	SER
1	D	416	SER
1	D	423	LYS
1	D	430	LEU
1	D	437	THR
1	D	444	LEU
1	D	453	ARG
1	D	458	GLU
1	D	483	LEU
1	D	485	ILE
1	D	486	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	299	HIS
1	A	309	HIS

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	352	HIS
1	A	374	GLN
1	A	375	HIS
1	A	390	GLN
1	B	31	GLN
1	B	106	HIS
1	B	374	GLN
1	B	390	GLN
1	C	31	GLN
1	C	168	ASN
1	C	170	HIS
1	C	299	HIS
1	C	312	ASN
1	C	390	GLN
1	C	447	GLN
1	D	31	GLN
1	D	106	HIS
1	D	299	HIS
1	D	312	ASN
1	D	390	GLN
1	D	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

39 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	501	-	3,3,3	0.54	0	2,2,2	0.25	0
2	EDO	A	502	-	3,3,3	0.52	0	2,2,2	0.24	0
2	EDO	A	503	-	3,3,3	0.55	0	2,2,2	0.15	0
2	EDO	A	504	-	3,3,3	0.45	0	2,2,2	0.47	0
2	EDO	A	505	-	3,3,3	0.61	0	2,2,2	0.18	0
2	EDO	A	506	-	3,3,3	0.47	0	2,2,2	0.39	0
2	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.33	0
3	C8E	A	508	-	20,20,20	0.44	0	19,19,19	0.45	0
2	EDO	B	501	-	3,3,3	0.52	0	2,2,2	0.33	0
2	EDO	B	502	-	3,3,3	0.40	0	2,2,2	0.41	0
2	EDO	B	503	-	3,3,3	0.62	0	2,2,2	0.16	0
2	EDO	B	504	-	3,3,3	0.69	0	2,2,2	0.14	0
2	EDO	B	505	-	3,3,3	0.47	0	2,2,2	0.39	0
2	EDO	B	506	-	3,3,3	0.37	0	2,2,2	0.40	0
2	EDO	B	507	-	3,3,3	0.52	0	2,2,2	0.25	0
2	EDO	B	508	-	3,3,3	0.66	0	2,2,2	0.10	0
2	EDO	B	509	-	3,3,3	0.52	0	2,2,2	0.31	0
2	EDO	B	511	-	3,3,3	0.49	0	2,2,2	0.43	0
3	C8E	B	512	-	20,20,20	0.35	0	19,19,19	0.66	0
2	EDO	C	501	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	C	502	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	C	503	-	3,3,3	0.48	0	2,2,2	0.28	0
2	EDO	C	504	-	3,3,3	0.60	0	2,2,2	0.23	0
2	EDO	C	505	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	C	506	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	C	507	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	C	508	-	3,3,3	0.49	0	2,2,2	0.39	0
3	C8E	C	509	-	20,20,20	0.41	0	19,19,19	0.77	0
2	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.39	0
2	EDO	D	502	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	D	503	-	3,3,3	0.55	0	2,2,2	0.19	0
2	EDO	D	504	-	3,3,3	0.53	0	2,2,2	0.19	0
2	EDO	D	505	-	3,3,3	0.52	0	2,2,2	0.28	0
2	EDO	D	506	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	D	507	-	3,3,3	0.50	0	2,2,2	0.19	0
2	EDO	D	508	-	3,3,3	0.50	0	2,2,2	0.39	0
2	EDO	D	509	-	3,3,3	0.48	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	510	-	3,3,3	0.52	0	2,2,2	0.65	0
3	C8E	D	511	-	20,20,20	0.47	0	19,19,19	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	501	-	-	0/1/1/1	0/0/0/0
2	EDO	A	502	-	-	0/1/1/1	0/0/0/0
2	EDO	A	503	-	-	0/1/1/1	0/0/0/0
2	EDO	A	504	-	-	0/1/1/1	0/0/0/0
2	EDO	A	505	-	-	0/1/1/1	0/0/0/0
2	EDO	A	506	-	-	0/1/1/1	0/0/0/0
2	EDO	A	507	-	-	0/1/1/1	0/0/0/0
3	C8E	A	508	-	-	0/18/18/18	0/0/0/0
2	EDO	B	501	-	-	0/1/1/1	0/0/0/0
2	EDO	B	502	-	-	0/1/1/1	0/0/0/0
2	EDO	B	503	-	-	0/1/1/1	0/0/0/0
2	EDO	B	504	-	-	0/1/1/1	0/0/0/0
2	EDO	B	505	-	-	0/1/1/1	0/0/0/0
2	EDO	B	506	-	-	0/1/1/1	0/0/0/0
2	EDO	B	507	-	-	0/1/1/1	0/0/0/0
2	EDO	B	508	-	-	0/1/1/1	0/0/0/0
2	EDO	B	509	-	-	0/1/1/1	0/0/0/0
2	EDO	B	511	-	-	0/1/1/1	0/0/0/0
3	C8E	B	512	-	-	0/18/18/18	0/0/0/0
2	EDO	C	501	-	-	0/1/1/1	0/0/0/0
2	EDO	C	502	-	-	0/1/1/1	0/0/0/0
2	EDO	C	503	-	-	0/1/1/1	0/0/0/0
2	EDO	C	504	-	-	0/1/1/1	0/0/0/0
2	EDO	C	505	-	-	0/1/1/1	0/0/0/0
2	EDO	C	506	-	-	0/1/1/1	0/0/0/0
2	EDO	C	507	-	-	0/1/1/1	0/0/0/0
2	EDO	C	508	-	-	0/1/1/1	0/0/0/0
3	C8E	C	509	-	-	0/18/18/18	0/0/0/0
2	EDO	D	501	-	-	0/1/1/1	0/0/0/0
2	EDO	D	502	-	-	0/1/1/1	0/0/0/0
2	EDO	D	503	-	-	0/1/1/1	0/0/0/0
2	EDO	D	504	-	-	0/1/1/1	0/0/0/0
2	EDO	D	505	-	-	0/1/1/1	0/0/0/0
2	EDO	D	506	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	507	-	-	0/1/1/1	0/0/0/0
2	EDO	D	508	-	-	0/1/1/1	0/0/0/0
2	EDO	D	509	-	-	0/1/1/1	0/0/0/0
2	EDO	D	510	-	-	0/1/1/1	0/0/0/0
3	C8E	D	511	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	EDO	3	0
2	A	504	EDO	4	0
2	A	505	EDO	1	0
2	A	506	EDO	1	0
3	A	508	C8E	9	0
2	B	502	EDO	6	0
2	B	504	EDO	1	0
2	B	505	EDO	3	0
2	B	506	EDO	6	0
2	B	508	EDO	4	0
3	B	512	C8E	16	0
2	C	501	EDO	9	0
2	C	502	EDO	1	0
2	C	504	EDO	4	0
2	C	505	EDO	1	0
2	C	506	EDO	1	0
3	C	509	C8E	12	0
2	D	502	EDO	1	0
2	D	503	EDO	3	0
2	D	504	EDO	1	0
2	D	506	EDO	1	0
2	D	507	EDO	1	0
2	D	508	EDO	1	0
2	D	510	EDO	1	0
3	D	511	C8E	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	436/486 (89%)	0.12	15 (3%)	49 58	31, 53, 85, 153	0
1	B	437/486 (89%)	0.06	17 (3%)	43 52	25, 44, 79, 139	0
1	C	438/486 (90%)	0.15	18 (4%)	41 50	27, 50, 92, 144	0
1	D	436/486 (89%)	0.17	20 (4%)	36 45	34, 56, 91, 133	0
All	All	1747/1944 (89%)	0.12	70 (4%)	42 51	25, 51, 88, 153	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	SER	5.0
1	C	485	ILE	4.5
1	D	486	THR	3.8
1	D	485	ILE	3.8
1	C	28	LYS	3.7
1	B	485	ILE	3.7
1	D	342	SER	3.6
1	D	343	THR	3.5
1	B	248	PRO	3.4
1	C	158	VAL	3.3
1	B	416	SER	3.2
1	A	341	ASP	3.1
1	D	321	ILE	3.1
1	A	344	ASP	3.1
1	D	28	LYS	3.0
1	D	248	PRO	3.0
1	D	291	ALA	2.9
1	D	316	LEU	2.9
1	B	415	SER	2.8
1	A	378	ASN	2.8
1	A	343	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	19	TRP	2.7
1	C	177	ILE	2.7
1	C	416	SER	2.6
1	C	27	ILE	2.6
1	A	403	ARG	2.6
1	C	180	SER	2.6
1	A	226	GLN	2.6
1	A	117	ASN	2.6
1	D	78	ARG	2.6
1	B	486	THR	2.5
1	C	405	SER	2.5
1	D	292	THR	2.5
1	C	223	ASP	2.5
1	A	280	SER	2.5
1	B	28	LYS	2.5
1	B	101	THR	2.4
1	D	441	ALA	2.3
1	C	389	VAL	2.3
1	C	487	PHE	2.3
1	A	222	GLU	2.3
1	D	181	GLN	2.3
1	B	27	ILE	2.3
1	C	224	VAL	2.2
1	A	340	GLU	2.2
1	B	175	ILE	2.2
1	C	119	ASP	2.2
1	D	158	VAL	2.2
1	B	226	GLN	2.2
1	B	211	HIS	2.2
1	A	45	VAL	2.1
1	A	177	ILE	2.1
1	C	248	PRO	2.1
1	C	211	HIS	2.1
1	B	158	VAL	2.1
1	D	45	VAL	2.1
1	B	249	ARG	2.1
1	B	250	ALA	2.1
1	C	175	ILE	2.1
1	C	205	PRO	2.1
1	B	98	ILE	2.1
1	C	226	GLN	2.1
1	B	182	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	296	LEU	2.0
1	D	378	ASN	2.0
1	A	293	ALA	2.0
1	B	106	HIS	2.0
1	D	221	ARG	2.0
1	D	296	LEU	2.0
1	D	290	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	A	504	4/4	0.77	0.34	15.50	54,54,54,54	0
2	EDO	D	504	4/4	0.62	0.29	10.65	68,68,68,68	0
2	EDO	C	508	4/4	0.66	0.45	9.48	82,82,82,82	0
2	EDO	B	506	4/4	0.94	0.26	7.61	42,42,42,42	0
2	EDO	C	505	4/4	0.87	0.21	6.72	60,60,60,60	0
2	EDO	D	505	4/4	0.56	0.40	6.65	91,91,91,91	0
2	EDO	B	508	4/4	0.81	0.38	6.46	58,58,58,58	0
2	EDO	A	503	4/4	0.70	0.34	4.74	65,65,65,65	0
2	EDO	B	511	4/4	0.89	0.23	4.61	71,71,71,71	0
2	EDO	B	503	4/4	0.72	0.33	3.70	56,56,56,56	0
2	EDO	C	504	4/4	0.85	0.26	3.53	51,51,51,51	0
2	EDO	B	505	4/4	0.96	0.26	3.02	45,45,45,45	0
2	EDO	B	501	4/4	0.88	0.25	2.62	62,62,62,62	0
2	EDO	A	505	4/4	0.71	0.23	2.37	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	D	502	4/4	0.85	0.30	2.32	71,71,71,71	0
3	C8E	A	508	21/21	0.86	0.27	2.26	66,66,66,66	0
3	C8E	B	512	21/21	0.94	0.22	2.17	42,42,42,42	0
2	EDO	C	502	4/4	0.94	0.24	2.17	59,59,59,59	0
2	EDO	D	510	4/4	0.84	0.22	1.66	57,57,57,57	0
2	EDO	B	509	4/4	0.82	0.22	1.12	62,62,62,62	0
3	C8E	C	509	21/21	0.95	0.17	0.91	42,42,42,42	0
3	C8E	D	511	21/21	0.93	0.20	0.77	65,65,65,65	0
2	EDO	D	508	4/4	0.94	0.16	0.50	67,67,67,67	0
2	EDO	D	507	4/4	0.94	0.12	0.48	44,44,44,44	0
2	EDO	C	507	4/4	0.96	0.11	0.35	38,38,38,38	0
2	EDO	D	503	4/4	0.94	0.14	0.32	49,49,49,49	0
2	EDO	C	503	4/4	0.96	0.15	-0.35	57,57,57,57	0
2	EDO	B	504	4/4	0.95	0.09	-0.65	38,38,38,38	0
2	EDO	A	501	4/4	0.96	0.08	-1.71	45,45,45,45	0
2	EDO	C	506	4/4	0.86	0.45	-	63,63,63,63	0
2	EDO	A	506	4/4	0.83	0.27	-	72,72,72,72	0
2	EDO	B	502	4/4	0.93	0.20	-	48,48,48,48	0
2	EDO	A	507	4/4	0.83	0.21	-	84,84,84,84	0
2	EDO	B	507	4/4	0.78	0.31	-	67,67,67,67	0
2	EDO	D	506	4/4	0.68	0.38	-	83,83,83,83	0
2	EDO	D	501	4/4	0.82	0.19	-	78,78,78,78	0
2	EDO	D	509	4/4	0.64	0.25	-	85,85,85,85	0
2	EDO	C	501	4/4	0.92	0.24	-	53,53,53,53	0
2	EDO	A	502	4/4	0.77	0.22	-	74,74,74,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.